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FROM QUANTUM CELLULAR AUTOMATA TO QUANTUM LATTICE GASES

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ABSTRACT

A natural architecture for nanoscale quantum computation is that of a quantum cellular automaton. Motivated by this observation, in this paper we begin an investigation of exactly unitary cellular automata. After proving that there can be no nontrivial, homogeneous, local, unitary, scalar cellular automaton in one dimension, we weaken the homogeneity condition and show that there are nontrivial, exactly unitary, partitioning cellular automata. We find a one parameter family of evolution rules which are best interpreted as those for a one particle quantum automaton. This model is naturally reformulated as a two component cellular automaton which we demonstrate to limit to the Dirac equation. We describe two generalizations of this automaton, the second of which, to multiple interacting particles, is the correct definition of a quantum lattice gas.

KEY WORDS: quantum cellular automaton; quantum lattice gas; quantum computation.

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1. Introduction

The realization that incentives to develop smaller and faster computers will eventually drive the devices from which they are constructed into the quantum regime motivated research into quantum mechanical limitations on deterministic computation as early as the 1970s [1]. The subsequent conceptions of universal quantum simulator by Feynman [2] and quantum Turing machine by Deutsch [3] initiated a series of investigations [4] into how aspects of quantum mechanics, specifically superposition and interference, might be exploited for computational purposes. Shor's remarkable discovery of a polynomial time quantum algorithm for factorization [5] (and the centrality of the factoring problem to modern cryptography [6]) has led to redoubled interest in the design and construction of quantum computational nanodevices [7]. It should be emphasized that the goal here is a computational device which will run *quantum* algorithms, not a quantum device which will run deterministic [8,9] or probabilistic [10] algorithms.

For a variety of reasons—the wire and gain problems, and the pragmatic observation that an array of simple devices is often easier to design and build than a single, more complicated device—it seems likely that massive parallelism will optimize nanoscale computer architecture [11]. In this paradigm, a quantum computer is a quantum cellular automaton (QCA): the state of each simple device (cell) in the array depends on the states of the cells in some local neighborhood at the previous timestep. Unlike the original cellular automaton (CA) models for parallel computation of von Neumann and Ulam [12], where this dependence is deterministic or probabilistic, here the dependence is quantum mechanical: There is a (complex) probability amplitude for the transition to each possible state, subject to the condition that the evolution be unitary, so that the total probability—the sum of the norm squared of the amplitude of each configuration—is always one.

QCA, therefore, provide a laboratory for analyzing both potential quantum computer architectures and algorithms; this is the motivation for initiating our study of them in this paper. Computation motivated study of QCA seems to have originated with the interesting work of Grössing and Zeilinger [13]. Their models, however, are only approximately quantum mechanical because, they argue, "except for the trivial case, strictly local, unitary evolution *of the whole QCA array* is impossible" [14]. Consequently, they study CA whose evolution is both nonunitary [13] and, although 'probability' preserving, nonlinear [14]. In Section 2 we begin by proving the following precise version of their claim:

No-go Lemma. *In one dimension there exists no nontrivial, homogeneous, local, scalar QCA. More explicitly, every band r-diagonal unitary matrix which commutes with the 1-step translation matrix is also a translation matrix, times a phase.*

and then continue by showing that even a slight weakening of the homogeneity/translation invariance condition allows nontrivial unitary evolution. Thus we will reserve the adjective 'quantum' for CA with exactly unitary, nontrivial, local evolution, in contrast to the usage by Grössing, Zeilinger, *et al.* [13,14] and Lent and Tougaw [9]. These are the QCA which should best model truly quantum parallel architectures. In this paper we consider only the

one dimensional situation; but this is not irrelevant for computational complexity issues since reversible CA capable of universal computation exist in one dimension [15], and reversible deterministic CA are, of course, unitary.

Section 3 contains output from several simulations of one dimensional QCA. Simulation on a deterministic computer must inevitably be slow, but this is acceptable since our goal here is understanding rather than the solution of any specific problem. It is easy to see qualitative differences from the simulations of Grössing, Zeilinger, *et al.* [13,14]; in particular, our simulations display particle-like features.

The latter observation motivates our reinterpretation in Section 4 of the evolution rule of such a QCA as the scattering rule for a quantum particle automaton. In this form the model is equivalent to Feynman's path integral formulation for a Dirac particle [16]; it is straightforward to solve the model exactly and to give a physical interpretation to the parameter in the scattering rule.

A lattice gas [17] formulation of this quantum particle automaton would consist of an array of nodes occupied by left and/or right moving particles which jump to the next node at the next timestep. Since there is only *one* particle in the model the amplitudes for left and right moving particles at a given node may be combined into a two component field as in the one dimensional Dirac equation in the chiral representation. Formulated as such a two component QCA, our quantum particle automaton is unitarily equivalent to the quantum lattice Boltzmann equation of Succi and Benzi [18] and to the one dimensional version of Bialynicki-Birula's QCA [19]. Since a two component QCA evades the conclusion of the No-go Lemma, in Section 5 we find the most general homogeneous/translation invariant unitary evolution rules for a neighborhood of radius one. The lattice gas paradigm motivates another generalization, however, to multiple (interacting) quantum particles. This new system, described in Section 6, is a quantum lattice gas automaton (QLGA) and may be expected to be relevant for modelling parallel quantum architectures constructed from few electron devices.

As Landauer [20] and others [21] have emphasized, achieving practical quantum computation will be difficult for a variety of reasons. The most fundamental problem is decoherence [22,23], which destroys the delicate interference phenomena on which quantum algorithms such as Shor's [5] depend. In Section 7 we observe that this is among the important issues in quantum computation which can be investigated using these models and also remark on some related research directions.

2. Quantum cellular automata

A CA consists of a lattice L of *cells* together with a *field* $\phi : \mathbb{N} \times L \to S$, where $\mathbb{N}$ denotes the non-negative integers labelling timesteps and S is the set of possible *states* in which the field is valued. The field evolves according to some *local rule*, *i.e.*, ϕ satisfies a recurrence relation of the form

$$\phi_{t+1}(x) = f\big(\phi_t(x+e) \mid e \in E(t,x)\big), \tag{1}$$

where $E(t,x)$ is a set of lattice vectors defining local *neighborhoods* for the automaton.

In the Schrödinger picture of quantum mechanics the state of a system at time t is a *state vector* in some Hilbert space (see, *e.g.*, [24]). The state vector evolves locally and unitarily, *i.e.*,

$$\phi_{t+1} = U\phi_t, \tag{2}$$

where U is a *unitary* matrix (more precisely, operator: $UU^\dagger = I = U^\dagger U$). Thus, if the configuration space is discrete, and the Hilbert space has a computational basis $|x\rangle$, $x \in L$, it is natural to try to construct a QCA model where $\phi_t(x)$ is the (complex scalar) coefficient of $|x\rangle$ in ϕ_t and the local evolution rule (1) is the unitary evolution rule (2) in this basis. Notice that this forces the QCA to be *additive* in Wolfram's terminology [25], *i.e.*, (1) becomes

$$\phi_{t+1}(x) = \sum_{e\in E(t,x)} w(t,x+e)\phi_t(x+e), \tag{3}$$

where the coefficients $w(t,x+e)$ are constrained by the unitarity condition. If both $E(t,x)$ and $w(t,x+e)$ are independent of t and x, the CA is *homogeneous*.

In one dimension ϕ_t can be written as a column vector with ordered entries $\phi_t(x)$, in which case locality corresponds to U being band diagonal. If, furthermore, the QCA is homogeneous, U must be invariant under the action of the translation operator T on the lattice—the permutation matrix with 1s on the subdiagonal—and (2) becomes

$$\begin{pmatrix} \vdots \\ \phi_{t+1}(-1) \\ \phi_{t+1}(0) \\ \phi_{t+1}(+1) \\ \vdots \end{pmatrix} = \begin{pmatrix} \ddots & & & & & & \\ & w_{-r} & \dots & w_{+r} & & & \\ & & w_{-r} & \dots & w_{+r} & & \\ & & & w_{-r} & \dots & w_{+r} & \\ & & & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_t(-1) \\ \phi_t(0) \\ \phi_t(+1) \\ \vdots \end{pmatrix}, \tag{4}$$

where $w(t,x+e) \equiv w_e$. (With periodic boundary conditions, of course, the top and bottom r rows will wrap around.) Grössing and Zeilinger consider the case $r = 1$ but find no nontrivial unitary matrix U. More generally,

No-go Lemma. *In one dimension there exists no nontrivial, homogeneous, local, scalar QCA. More explicitly, every band r-diagonal unitary matrix U which commutes with the 1-step translation matrix T is also a translation matrix T^k for some $k \in \mathbb{Z}$, times a phase.*

Proof. When $r = 0$, $U = w_0 I$ and unitarity implies $|w_0|^2 = 1$ so U is the 0-step translation matrix (the identity) times a phase. Assume that the statement is true for $r-1$. For a 1-step translation invariant band r-diagonal matrix, unitarity implies:

$$\begin{aligned}
w_{-r}\bar{w}_{-r} + w_{-r+1}\bar{w}_{-r+1} + \cdots + w_{r-1}\bar{w}_{r-1} + w_r\bar{w}_r &= 1 && (5_{-r})\\
w_{-r+1}\bar{w}_{-r} \quad + \cdots + w_{r-1}\bar{w}_{r-2} + w_r\bar{w}_{r-1} &= 0 && (5_{-r+1})\\
&\vdots\\
w_{r-1}\bar{w}_{-r} \quad + w_r\bar{w}_{-r+1} &= 0 && (5_{r-1})\\
w_r\bar{w}_{-r} &= 0, && (5_r)
\end{aligned}$$

together with the complex conjugate equations. By equation (5_r), at least one of w_r and w_{-r} vanishes, say w_r. Then we may assume $w_{-r} \neq 0$; otherwise the conclusion follows immediately from the inductive hypothesis. But then equation (5_{r-1}) forces $w_{r-1} = 0$; ...; equation (5_{-r+1}) forces $w_{-r+1} = 0$; and equation (5_{-r}) becomes $|w_{-r}|^2 = 1$, *i.e.*, the only nonzero weight, w_{-r}, is a phase. Then $U = w_{-r}T^r$, where T^r is the r-step translation matrix. ■

CA which evolve simply by translation are not very interesting, so Grössing and Zeilinger relax the unitarity constraint, setting

$$w_{-1} = i\delta, \quad w_0 = 1, \quad w_{+1} = i\bar{\delta},$$

so that the evolution is only approximately unitary, with errors of $O(|\delta|^2)$ accumulating at each timestep [13]. Since the evolution is nonunitary, *quantum* probability is not preserved. Instead, all the amplitudes are normalized by an overall factor at each step to make $\sum_x |\phi_t(x)|^2 = 1$; this may be thought of as a nonlocal (and non-quantum mechanical) aspect of the evolution [14].

Our choice, instead, is to weaken the homogeneity condition but to insist still on exactly unitary, local evolution, thus maintaining consistency with standard quantum mechanics. The evolution matrix in (4) is 1-step translation invariant, *i.e.*, $TUT^{-1} = U$; a natural way to relax this constraint is to require $T^2UT^{-2} = U$, so that the evolution is only 2-step translation invariant. For $r = 1$ we have then:

$$U = \begin{pmatrix}
\ddots & & & & & & & \\
 & a & b & c & & & & \\
 & & d & e & f & & & \\
 & & & a & b & c & & \\
 & & & & d & e & f & \\
 & & & & & & & \ddots
\end{pmatrix},$$

and unitarity requires:

$$\begin{aligned}
a\bar{a} + b\bar{b} + c\bar{c} &= 1 \qquad & d\bar{d} + e\bar{e} + f\bar{f} &= 1\\
b\bar{d} + c\bar{e} &= 0 & e\bar{a} + f\bar{b} &= 0 \qquad (6)\\
c\bar{a} &= 0 & f\bar{d} &= 0,
\end{aligned}$$

together with the complex conjugate equations.

There are two types of solutions to these equations. The uninteresting ones have only a and d (or c and f) nonzero, both with norm 1; in this case the evolution is by translation and multiplication by alternating phases. The interesting solutions to (6) have $c = d = 0$ (or $a = f = 0$) and the matrix

$$S := \begin{pmatrix} e & f \\ a & b \end{pmatrix} \quad (\text{or } \begin{pmatrix} b & c \\ d & e \end{pmatrix}) \tag{7}$$

unitary; in this case U is block diagonal, each block acting only on a pair of adjacent cells.

Evolving by U at each timestep would partition the CA into a set of noninteracting systems each comprised of a pair of adjacent cells. Instead, we evolve by U and by TUT^{-1} at alternating timesteps, changing the pairing and allowing propagation. Such alternating evolution has been referred to as a *staggered* rule for a *checkerboard* model in the context of probabilistic CA and two dimensional statistical mechanics models [26], and as a *partitioning* CA in the context of reversible CA [27]. Since unitary evolution includes deterministic reversible evolution, the No-go Lemma applies in the latter context in one dimension (of course, the overall phase referred to in the statement of the lemma must be 1), and it is natural that triviality has been evaded there in the same way.

3. Simulations

The matrix $S \in U(2)$ may be parameterized as

$$S = \begin{pmatrix} e^{i\alpha} \sin\theta & e^{i\beta} \cos\theta \\ e^{i\gamma} \cos\theta & e^{i\delta} \sin\theta \end{pmatrix},$$

with $\alpha - \beta - \gamma + \delta \equiv \pi \pmod{2\pi}$. Rather than continuing in full generality, we shall impose parity invariance, which forces $b = e$ and $a = f$ (or $b = e$ and $c = d$) in (7). Dividing out an overall phase which is unobservable (*i.e.*, has no effect on probabilities), the cell pair evolution matrix S becomes

$$S = \begin{pmatrix} i \sin\theta & \cos\theta \\ \cos\theta & i \sin\theta \end{pmatrix}. \tag{8}$$

Simulation of a single timestep of this QCA is achieved by a series of matrix multiplications:

$$\begin{pmatrix} \phi_{t+1}(x-1) \\ \phi_{t+1}(x) \end{pmatrix} = \begin{pmatrix} i \sin\theta & \cos\theta \\ \cos\theta & i \sin\theta \end{pmatrix} \begin{pmatrix} \phi_t(x-1) \\ \phi_t(x) \end{pmatrix}, \tag{9}$$

for each $x \equiv t+1 \pmod 2$, say. Although these matrix multiplications commute since they evolve disjoint pairs of cells, sequential simulation of this intrinsically parallel evolution will be slow, as it always is for CA. Furthermore, since the field values and the evolution parameters are complex numbers, the usual efficiencies of bitwise computation are unavailable. Nevertheless, simulation of small systems is easy and informative; an additional, more serious difficulty will not appear until the simulations of QLGA in Section 5.

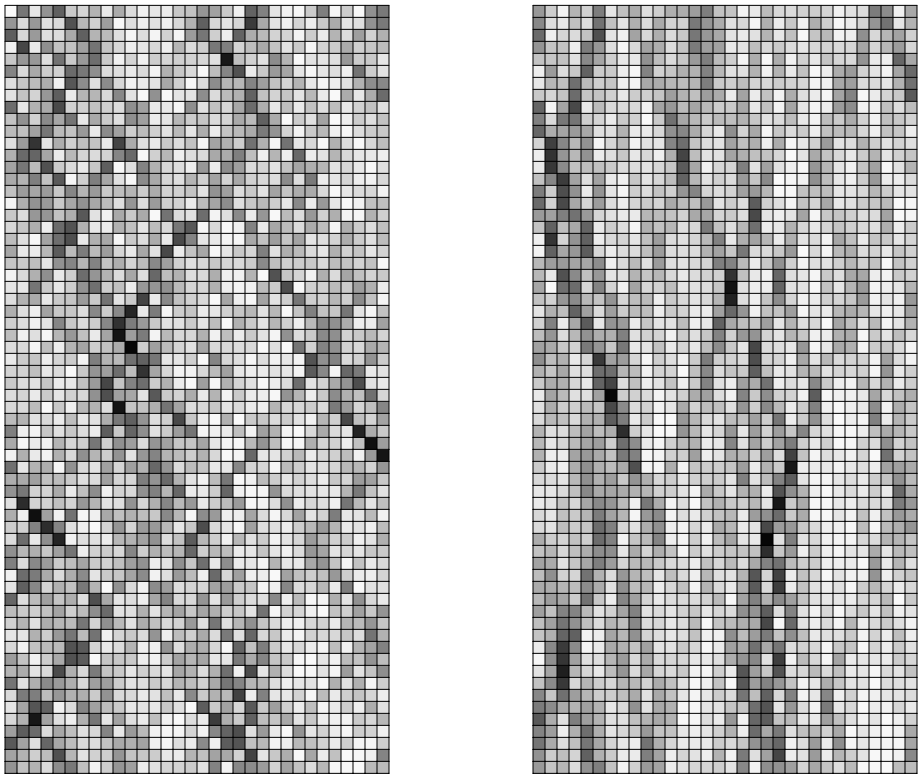

Figure 1. Two simulations of the $r = 1$ QCA starting with the same initial conditions. On the left $\theta = \pi/6$ and on the right $\theta = \pi/3$. Time runs upward and periodic boundary conditions have been imposed.

Figure 1 shows simulations of our QCA for $\theta = \pi/6$ and $\theta = \pi/3$, starting from the same random initial condition. The darkness of each cell is (positively) proportional to its probability, *i.e.*, the norm squared of its amplitude (field value), and it appears that there is a probability flow in each case, slower for $\theta = \pi/3$. This is expected since for $\theta = \pi/2$, U is proportional to the identity (the overall factor of i is unobservable) and there is no flow, while for $\theta = 0$, S simply interchanges the states of adjacent cells so that probability propagates with speed 1 in lattice units.

Starting with the simplest symmetric initial condition demonstrates the probability propagation more clearly. In the simulation shown in Figure 2, the initial condition is

$$\phi(x) = \begin{cases} 1/\sqrt{2} & \text{if } x \in \{15, 16\}; \\ 0 & \text{otherwise.} \end{cases}$$

Here $\theta = \pi/4$. Measuring the locations of the two peaks of the probability distribution at successive timesteps indicates that the propagation speed is approximately $2/3$ in lattice units.

This is consistent with the evolution of the even simpler initial condition shown in Figure 3. Here the only nonzero initial value is at $x = 0$. Again $\theta = \pi/4$ and the propagation speed still appears to be approximately $2/3$ in lattice units. In both of these simulations

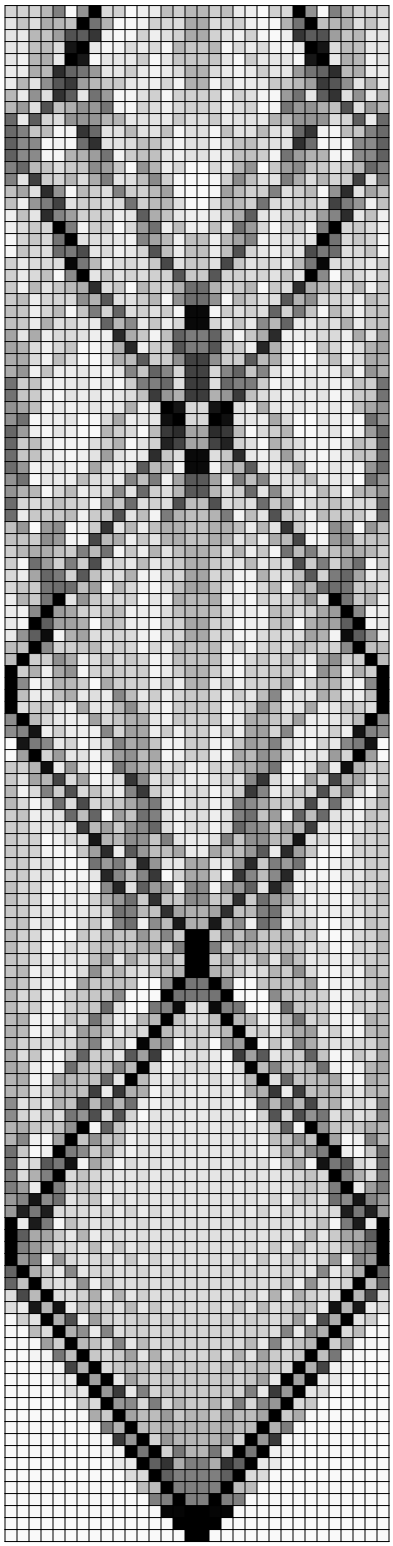

Figure 2. The $r = 1$ QCA with $\theta = \pi/4$ and equal initial nonzero amplitudes at $x = 15, 16$.

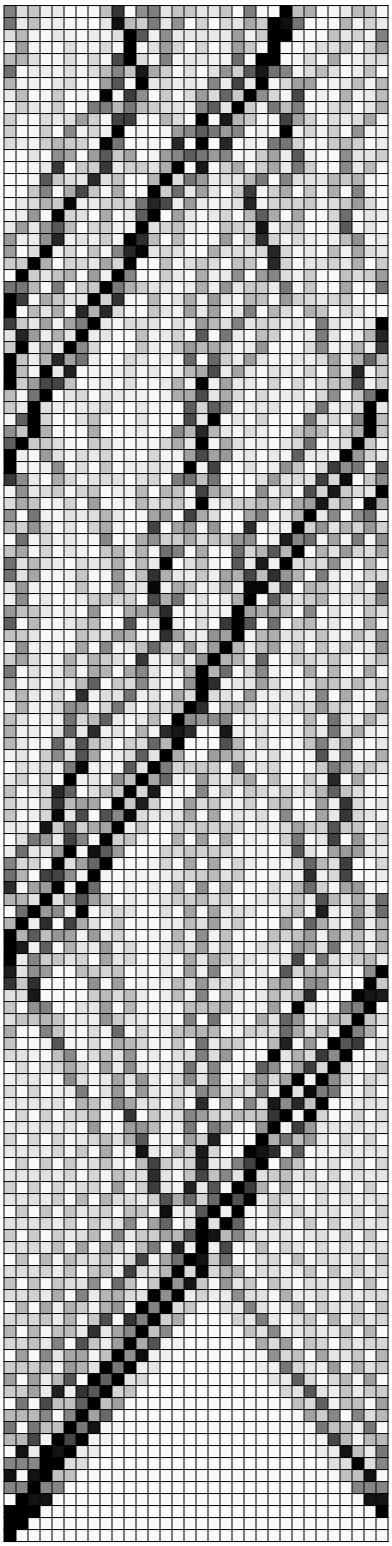

Figure 3. The same QCA with initial nonzero amplitude only at $x = 0$.

there are peaks in the probability distribution which remain substantially localized for the duration of the evolution shown. This behavior, particularly in the symmetric simulation shown in Figure 2, should be contrasted with the results of Grössing, Zeilinger, *et al.* [13,14], which demonstrate quite different qualitative features: In their simulations macroscopic patterns develop and there is nothing which has the particle-like appearance of the persistent localized peaks in these probability distributions.

4. Quantum particle automata

The underlying particle nature of this alternating/partitioning QCA can be seen on the *trajectory lattice* dual to the spacetime lattice of the CA. As shown in Figure 4, each adjacent pair of cells acted on by S has a dual pair of spacetime edges which intersect and then continue along the same trajectories at the next timestep, becoming the spacetime edges dual to the same pair of cells. On the spacetime trajectory lattice the alternating action of what should now be called the *scattering matrix* S is automatic; the values of ϕ are attached to the edges of the trajectory lattice and undergo a unitary transformation by S at each vertex.

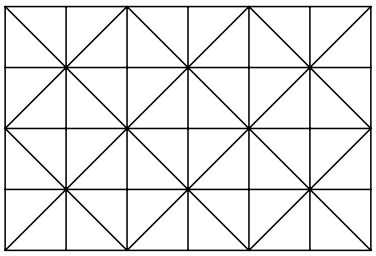

Figure 4. The spacetime CA lattice is the rectangular array of square cells; the dual particle trajectory lattice consists of the diagonal edges.

The value of ϕ on a left/right pointing edge of the trajectory lattice should be interpreted as the amplitude for a left/right moving particle being there. That is, equation (9) means that if there is a right moving particle at time t, at time $t+1$ it either becomes a left moving particle with amplitude $i\sin\theta$ or continues moving right with amplitude $\cos\theta$. In particular, if there is some nonzero amplitude on each of two intersecting right and left going edges of the trajectory lattice, they may be evolved independently and then added. There is no interaction, so this is effectively a model of a *single* particle; the QCA is a *quantum particle automaton*. $\phi_t(x)$ is the amplitude for the particle being in state $|x\rangle$ during the time interval $(t,t+1)$, where, if x takes integer values on the vertical lines in Figure 4,

$$|x\rangle := \begin{cases} \textit{left} \text{ moving from } x+1 & \text{if } t \not\equiv x \pmod 2 \\ \textit{right} \text{ moving from } x & \text{if } t \equiv x \pmod 2. \end{cases} \tag{10}$$

That is, the computational basis $|x\rangle$ is a set of eigenstates of an operator measuring more than just position. Projecting onto the position subspace adds (incoherently, *i.e.*, the *probabilities* add) the amplitudes for left and right movers existing at (t,x), for $t \equiv x \pmod 2$, and gives a much clearer picture of the evolution. Figures 5 and 6 show this representation of the simulations of Figures 2 and 3, respectively. Since the evolution lies within the 'lightcone', *i.e.*, the propagation speed is less that 1 in lattice units, Figures 5 and 6 are in lightcone coordinates:

$$u := \big(t + (x - x_0)\big)/2$$
$$v := \big(t - (x - x_0)\big)/2,$$

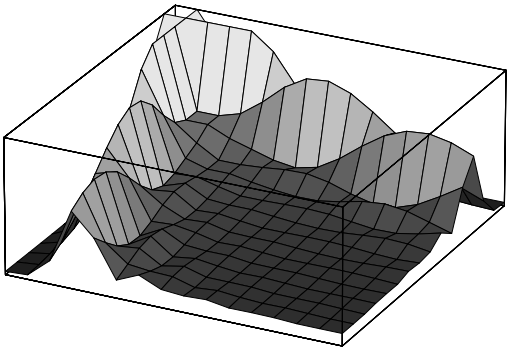

Figure 5. Position measurements in lightcone coordinates for the QCA of Figure 2. The probability 1 measurement at $(0,0)$ has been clipped.

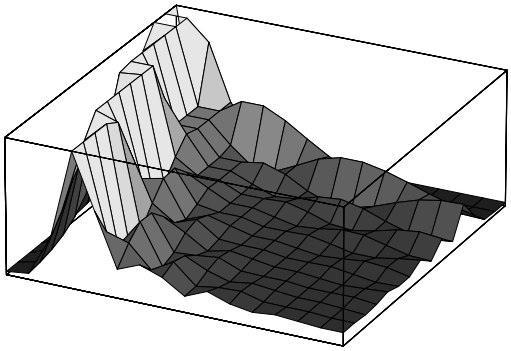

Figure 6. The same representation of the QCA of Figure 3. The first few (large) probabilities in the evolution have been clipped.

where x_0 implements a translation of the origin: by 16 in Figure 5 and by 0 in Figure 6. In both figures only the spacetime region covered by $0 \leq u, v \leq 16$ is shown, the origin is at the rear corner, and time runs forward to the front corner. The parity dependence (visible in the patterns of alternating dark and light cells) in Figures 2 and 3 has been smoothed out in these so that both the probable particle trajectories as well as their wave-like character are clearly visible.

That the solution is as smooth as shown here suggests that the quantum particle automaton may be a discrete approximation to a continuum system, possibly with an exact solution. This is, in fact, the case. Although we have been led to it simply by the assumptions of discreteness, locality, and unitarity (and parity invariance), we will show that this quantum particle automaton is a discrete approximation to the Feynman path integral for a Dirac particle in one dimension [16]. Furthermore, it is exactly solvable, even without going to the continuum limit.

Consider a right moving particle at $(t,x) = (0,0)$, *i.e.*, $\phi_0(0) = 1$. The amplitude $\phi_t(x)$ for the particle being in state $|x\rangle$ at time t is defined to be the *propagator* $K(t,x;0,0)$. This is exactly the (coherent) sum of the amplitudes of all possible paths in the trajectory lattice from $(0,0)$ to (t,x)—the sum-over-histories, or Feynman path sum. Figure 7 shows two typical paths a right moving particle from $(0,0)$ might take, arriving in left moving state $|x-1\rangle$ or right moving state $|x\rangle$ just after time t ($\equiv x \pmod 2$). Each path consists of u steps right and v steps left, followed by the terminal step, and is

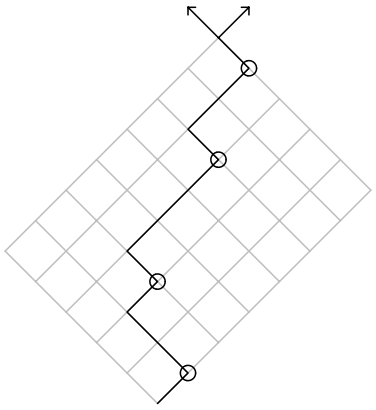

Figure 7. A typical initially right moving path from $(u,v) = (0,0)$ to $(7,5)$ with both left and right moving final steps and four right to left direction changes.

completely characterized by the locations of the right to left direction changes—the points circled in Figure 7. If there are k such direction changes, a path ending at $|x-1\rangle$ has amplitude

$$(i\sin\theta)^{2k-1}(\cos\theta)^{u+v-(2k-1)} = (\cos\theta)^{u+v}(i\tan\theta)^{2k-1} \tag{11}$$

and one ending at $|x\rangle$ has amplitude

$$(i\sin\theta)^{2k}(\cos\theta)^{u+v-2k} = (\cos\theta)^{u+v}(i\tan\theta)^{2k}. \tag{12}$$

Counting the numbers of paths with k direction changes and multiplying by the amplitudes in (11) and (12) gives

$$\begin{aligned}\phi_t(x-1) &= (\cos\theta)^{u+v}\cdot i\tan\theta\sum_{k=1}^{\infty}\binom{u-1}{k-1}\binom{v}{k-1}(i\tan\theta)^{2k-2}\\ &= (\cos\theta)^{u+v}\cdot i\tan\theta\,{}_2F_1(1-u,-v;1|-\tan^2\theta)\end{aligned} \tag{13}$$

and

$$\begin{aligned}\phi_t(x) &= (\cos\theta)^{u+v}\left[\delta(v)+\big(1-\delta(v)\big)\sum_{k=1}^{\infty}\binom{u}{k}\binom{v-1}{k-1}(i\tan\theta)^{2k}\right]\\ &= (\cos\theta)^{u+v}\Big[\delta(v)-\big(1-\delta(v)\big)u\tan^2\theta\,{}_2F_1(1-u,1-v;2|-\tan^2\theta)\Big],\end{aligned} \tag{14}$$

where the $\delta(v)$ term counts the single $k=0$ path which contributes only when $v=0$, and ${}_2F_1$ is the Gauss hypergeometric function. These amplitudes, together with those for an initially left moving path (which may be obtained from (13) and (14) by interchanging u and v), define $K(t,x;0,0)$ for the quantum particle automaton. By linearity (additivity), therefore, they provide an exact solution for the evolution of any initial condition.

Although Lorentz invariance is manifestly broken by the spacetime lattice, it is regained in the continuum limit: Let the lattice spacing be ϵ, *i.e.*, replace θ by $\epsilon\theta$ and (u,v) by $(u/\epsilon, v/\epsilon)$. Then for $u,v\neq 0$, as $\epsilon\to 0$,

$$\begin{aligned}\phi_t(x-1) &\sim i\tan\epsilon\theta\,{}_0F_1(-;1|-(uv/\epsilon^2)\tan^2\epsilon\theta)\\ &\sim i\epsilon\theta J_0(\tau\theta)\end{aligned} \tag{15}$$

and

$$\begin{aligned}\phi_t(x) &\sim -(u/\epsilon)\tan^2\epsilon\theta\,{}_0F_1(-;2|-(uv/\epsilon^2)\tan^2\epsilon\theta)\\ &\sim -(u\epsilon/\tau)J_1(\tau\theta),\end{aligned} \tag{16}$$

where ${}_0F_1$ is obtained by taking the confluent limit of ${}_2F_1$ twice [28], J_i is the ith order Bessel function of the first kind, and $\tau := 2\sqrt{uv} = \sqrt{t^2-x^2}$ is the spacetime separation of $(0,0)$ and (t,x). The limits (15) and (16), together with their initially left moving counterparts (still obtained by interchanging u and v), give exactly the continuum propagator for

the Dirac equation for a particle of mass θ [29]. When $\theta = 0$, the contributions from (15) and (16) vanish and the propagator has support only on the lightcone (the $\delta(v)$ term in (14)). These results explain our observations about the simulations shown in Figures 1, 2 and 3: For $\theta = 0$ the propagation is at speed 1 in lattice units (*i.e.*, is along the lightcone); as θ increases the 'mass' $\tan\theta$ increases and the speed decreases; when $\theta = \pi/2$,the 'mass' is infinite and there is no propagation.

5. Two component quantum cellular automata

In the chiral representation, the one dimensional Dirac equation describes the evolution of a two component complex spinor [29]. Although our interests in this paper are primarily to investigate possible QCA rather than to construct discrete models for fundamental physical processes [30], the results from the previous section indicate that in the quantum particle automaton it is natural to combine the amplitudes for the single particle leaving position x to the left and to the right into a two component field $\psi_t(x) := \big(\phi_t(x-1), \phi_t(x)\big)$ for $x \equiv t \pmod 2$ and motivate consideration of *two component* QCA. In terms of ψ, the evolution rule (9) becomes

$$\psi_{t+1}(x) = \begin{pmatrix} 0 & i\sin\theta \\ 0 & \cos\theta \end{pmatrix} \psi_t(x-1) + \begin{pmatrix} \cos\theta & 0 \\ i\sin\theta & 0 \end{pmatrix} \psi_t(x+1). \tag{17}$$

The most general local evolution rule for a two component QCA still has the form (3), with ϕ replaced by the two component field ψ defined at *all* cells and the coefficients w now representing 2×2 matrices. The evolution rule (17) for our quantum particle automaton already shows that the conclusion of the No-go Lemma can be evaded in a two component, one dimensional QCA; the issue becomes identifying all possible local, homogeneous, unitary evolution matrices U as in (4). For $r = 1$, the most general local evolution rule is

$$\psi_{t+1}(x) = w_{-1}\psi_t(x-1) + w_0\psi_t(x) + w_{+1}\psi_t(x+1) \tag{18}$$

and the unitarity constraints are still those given by equations (5_m):

$$w_{-1}w_{-1}^\dagger + w_0 w_0^\dagger \quad + w_{+1}w_{+1}^\dagger = I \tag{19_{-1}}$$
$$w_0 w_{-1}^\dagger + w_{+1}w_0^\dagger \quad = 0 \tag{19_0}$$
$$w_{+1}w_{-1}^\dagger = 0, \tag{19_{+1}}$$

together with their Hermitian conjugate equations.

Parity invariance imposes two additional constraints:

$$w_{-1} = P w_{+1} P^{-1} \tag{20}$$
$$w_0 = P w_0 P^{-1} \qquad \left(P := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right). \tag{21}$$

Equation (19_{+1}) implies that at least one of w_{-1} and w_{+1} is singular; by (20) both are, have the same eigenvalues, and hence can be simultaneously row/column reduced to, say,

$$w_{-1} = \begin{pmatrix} 0 & iae^{i\alpha} \\ 0 & be^{i\beta} \end{pmatrix} \qquad w_{+1} = \begin{pmatrix} be^{i\beta} & 0 \\ iae^{i\alpha} & 0 \end{pmatrix}. \tag{22}$$

That is, any parity invariant, $r = 1$, one dimensional, two component QCA is unitarily equivalent to one with w_{-1} and w_{+1} in the form (22). Equation (21) implies

$$w_0 = \begin{pmatrix} ce^{i\gamma} & ide^{i\delta} \\ ide^{i\delta} & ce^{i\gamma} \end{pmatrix}. \tag{23}$$

Using the forms (22) and (23) in equation (19_0) shows that $\gamma = \alpha$, $\delta = \beta$, and $d = -cb/a$. Finally, equation (19_{-1}) forces

$$a^2 + b^2 + c^2(1 + b^2/a^2) = 1$$

and shows that the only nonzero solution occurs when $\alpha = \beta$. Thus we may factor out an overall phase and reparameterize to find that any nontrivial solution to equations (19_m), (20) and (21) is unitarily equivalent to

$$\begin{gathered} w_{-1} = \cos\rho \begin{pmatrix} 0 & i\sin\theta \\ 0 & \cos\theta \end{pmatrix} \qquad w_{+1} = \cos\rho \begin{pmatrix} \cos\theta & 0 \\ i\sin\theta & 0 \end{pmatrix} \\ w_0 = \sin\rho \begin{pmatrix} \sin\theta & -i\cos\theta \\ -i\cos\theta & \sin\theta \end{pmatrix}. \end{gathered} \tag{24}$$

Our quantum particle automaton, with evolution rule given by (17), is the most general $\rho = 0$ solution; the one dimensional lattice Boltzmann equation of Succi and Benzi [18] is unitarily equivalent to ours, as is the one dimensional version of Bialynicki-Birula's unitary CA for the Dirac equation [19]. As two component QCA with $\rho = 0$, each of these models consists of a pair of independent automata supported on the spacetime cells $t + x \equiv 0$ and 1 (mod 2), respectively. Setting $\rho \not\equiv 0 \pmod{\pi}$ couples these two automata. Figure 8 shows two simulations of a particle initially localized to be right moving from $x = 0$, evolving with the same value of θ, but different values of ρ. Cell darkness is (positively) proportional to the probability $\psi^\dagger\psi$, where $\psi^\dagger$ is the conjugate transpose of ψ. Increasing the coupling ρ towards $\pi/2$ has the expected effect of decreasing the propagation speed.

6. Quantum lattice gas automata

Having reinterpreted our original QCA (9) as a quantum particle automaton (17), the lattice gas paradigm [17] suggests a different generalization than the two component QCA with evolution rule (18), namely to *multiple* particles. A LGA is a CA in which the possible states of the field are taken to represent occupation by α-moving particles. The evolution rule consists of two stages: each particle at x jumps to $x + \alpha$ and then the particles now at x interact to possibly change their directions of motion.

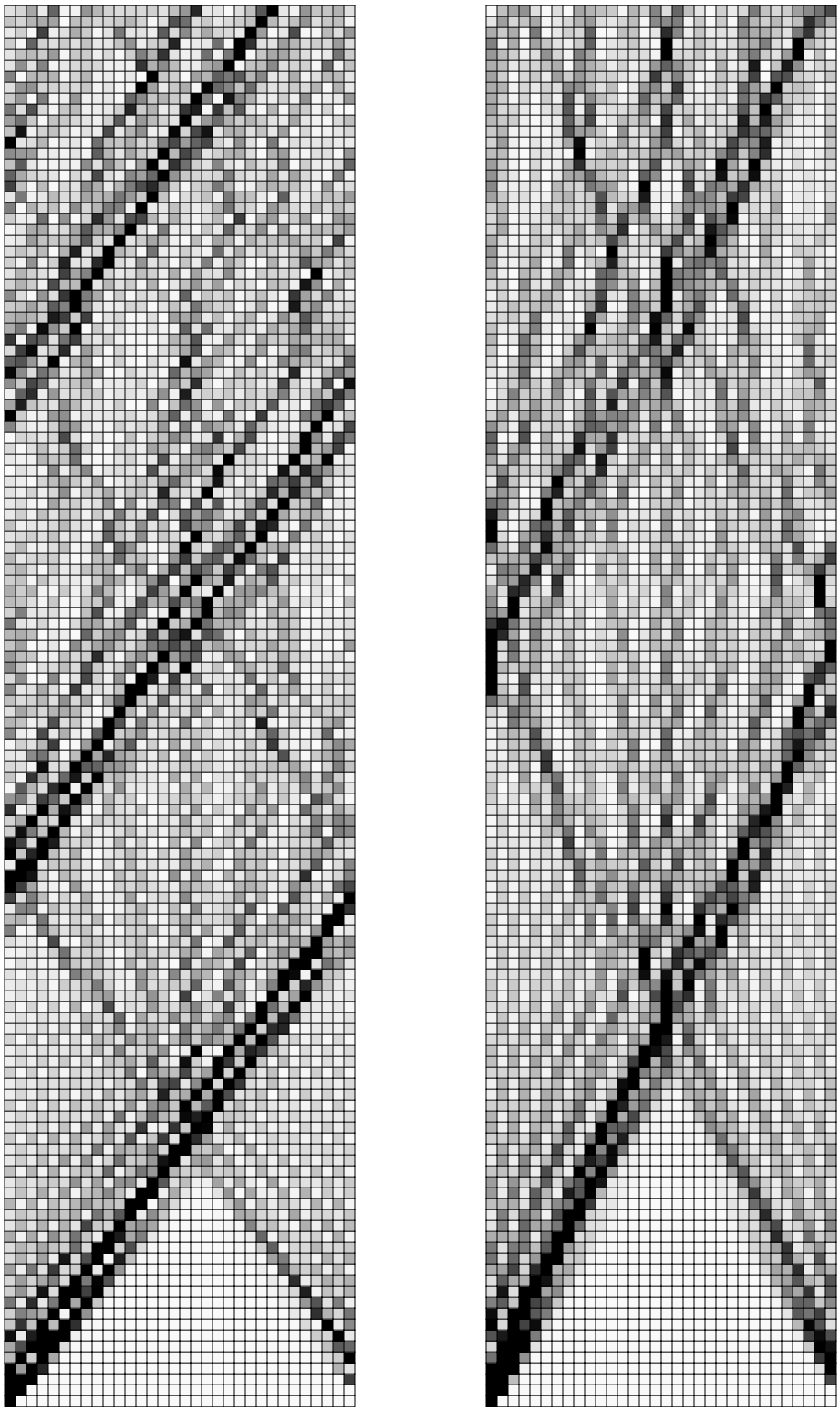

Figure 8. Two simulations of the $r = 1$ two component QCA starting with the same initial conditions. In both, $\theta = \pi/4$, while $\rho = \pi/6$ on the left and $\pi/3$ on the the right.

In the single particle interpretation of our QCA developed in Section 4, the wave function $\phi_t = \sum_x \phi_t(x)|x\rangle$ describes the quantum state of the system at time t, where $|x\rangle$ is the one particle state defined in (10). The scattering matrix S given in (8) may be taken to act on the basis states $|x\rangle$ rather than on the coefficient amplitudes $\phi_t(x)$:

$$S|x\rangle_t = \begin{cases} \cos\theta\,|x-1\rangle_{t+1} + i\sin\theta\,|x\rangle_{t+1} & t \not\equiv x \pmod 2 \\ i\sin\theta\,|x\rangle_{t+1} + \cos\theta\,|x+1\rangle_{t+1} & t \equiv x \pmod 2. \end{cases}$$

That is, the left (right) moving particle jumps to the left (right) and either continues in the same direction with amplitude $\cos\theta$ or reverses direction with amplitude $i\sin\theta$; this is exactly the form of a (quantum) LGA evolution rule.

Generalization to multiple particles has both kinematical and dynamical aspects [31]: The Hilbert space must be extended to have basis states $|x_1,\ldots,x_n\rangle$ (denoting the configuration with n particles in states $x_1,\ldots,x_n$). The familiar restriction in classical LGA to occupation numbers 0 and 1, *i.e.*, an *exclusion principle*, is consistent with the fermionic character of the Dirac equation we found in the macroscopic limit of the quantum particle automaton. With this constraint the Hilbert space has dimension 2^N (if it is N for the corresponding QCA) since no two of the x_i in a basis state may be identical. Each particle still jumps at each timestep, but now there is the possibility that two particles (although no more than two if the exclusion principle is in effect) will jump to the same position at the same time. Thus the scattering matrix S must also be extended to include amplitudes S_{ij} for the transitions $i \leftarrow j$ where $00 \le i,j \le 11$ (in binary) and the position of the 1s in an index indicates the occupied particle states in the pair of cells (the position) under consideration. Retaining parity invariance from the one particle model and imposing particle number conservation, the most general local evolution rule is defined by the scattering matrix

$$S = \begin{array}{c} \\ \nearrow \\ \nwarrow \\ \nwarrow\nearrow \end{array} \begin{array}{c} \begin{array}{cccc} \nwarrow & \nearrow & & \nearrow\nwarrow \end{array} \\ \begin{pmatrix} a & & & \\ & b & c & \\ & c & b & \\ & & & f \end{pmatrix} \end{array},$$

which, just as in Section 2, must be unitary to ensure unitary evolution of the whole automaton. Dividing out an overall phase, S may be parameterized as

$$S = \begin{pmatrix} 1 & & & \\ & ie^{i\alpha}\sin\theta & e^{i\alpha}\cos\theta & \\ & e^{i\alpha}\cos\theta & ie^{i\alpha}\sin\theta & \\ & & & e^{i\beta} \end{pmatrix}. \tag{25}$$

Thus individual particles evolve just as before except for a multiplicative phase of $e^{i\alpha}$ at each timestep, unless two jump to the same position at the same time, in which case they exit multiplied by the phase $e^{i\beta}$. This is the simplest QLGA in one dimension.

To simulate a deterministic or probabilistic LGA, it is sufficient to store only a single particle configuration at each timestep and then evolve it to the next with the appropriate

probability (1 in the deterministic case). Each run produces a single final configuration; multiple runs produce the same probability distribution of final configurations as would computing the whole Markov process, *i.e.*, multiplying a vector representing state probabilities by the Markov evolution matrix analogous to U. Because probabilities do not add in the quantum situation—there is interference in the coherent sum of amplitudes—only the latter procedure is viable for a QLGA. For QLGA the dimension of the Hilbert space is exponential in the cardinality N of the lattice, so simulation is potentially exponentially slower than for deterministic/probabilistic LGA. With particle number conservation, however, the problem is not completely intractable: for n fermionic particles the Hilbert (or Fock, as it would be called in the quantum field theory context) space has dimension $\binom{N}{n}$; when $n = 1$ this is just the N amplitudes computed at each step in the one particle simulations of Figures 1, 2, 3 and 8.

Figure 9 shows the next simplest situation, a QLGA with $n = 2$ interacting particles. Since one might expect that an interaction consisting only of phase multiplication (the $e^{i\beta}$ term in S) would have little effect, Figure 9 compares the two particle simulation with particles initially at $x = 4$ (right moving) and $x = 11$ (left moving) to a one particle simulation with the particle initially at $x = 4$ and $x = 11$ with equal amplitude. In each simulation cell darkness is (positively) proportional to the probability that a particle is present. The qualitative difference is immediately apparent.

The difficulty of simulating the n particle sector of the Fock space clearly grows polynomially with $n \ll N$. But note that there is a duality between the particles and the 'holes' (the unoccupied states) which suggests that they should be considered to be *antiparticles*—not surprising since we saw in Section 4 that the one particle sector limits to the Dirac equation. In fact, the scattering matrix (25) is the Minkowski space form of the Boltzmann weight in the symmetric six-vertex model, which is itself a specialization of the Boltzmann weight for the eight-vertex model:

$$S = \begin{array}{c} \\ \searrow\nearrow \\ \searrow\nearrow \\ \nwarrow\swarrow \\ \nwarrow\nearrow \end{array} \begin{array}{c} \begin{array}{cccc} \swarrow\searrow & \swarrow\nwarrow & \nearrow\searrow & \nearrow\nwarrow \end{array} \\ \begin{pmatrix} a & & & d \\ & b & c & \\ & c & b & \\ d & & & a \end{pmatrix} \end{array},$$

where the downward pointing arrows represent the antiparticles (the CP duals) of the original particles. Not only are these models exactly solvable [32], but in the appropriate limit (critical point) the Minkowski space symmetric six-vertex model becomes the massive Thirring model [33]. As usual, of course, exactly solvable does not mean that expectation values of all observables can be computed; even in the restricted parameter domain corresponding to probabilistic evolution only certain correlation functions have been computed [34]. This leaves a wide range of problems which may be most easily solved by simulation with this QLGA.

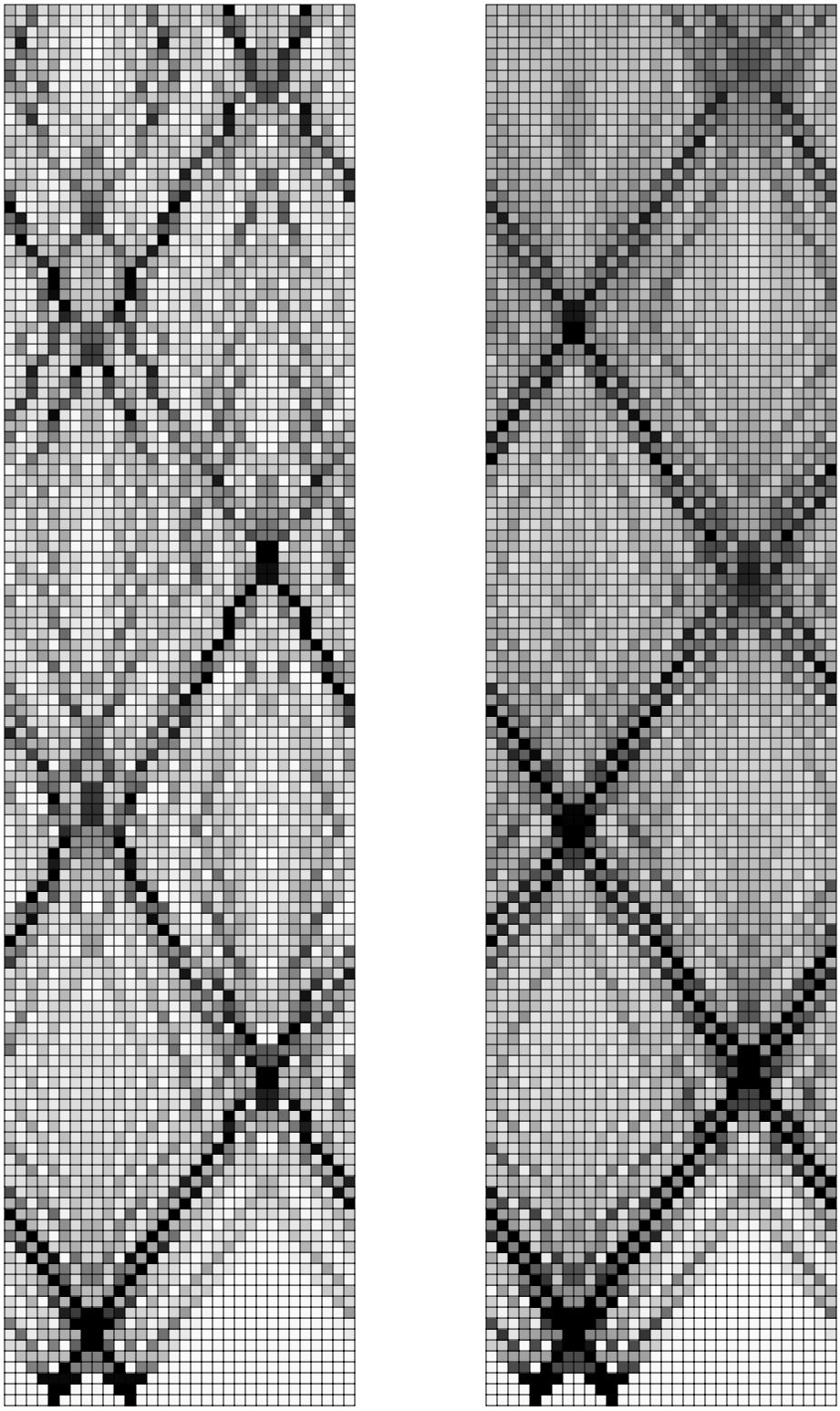

Figure 9. The QLGA with scattering matrix (25). The simulation on the left contains a single particle initially at $x = 4$ and $x = 11$ with equal amplitude. The one on the right contains two particles, initially at $x = 4$ and $x = 11$. In both simulations $\theta = \pi/4$, $\alpha = 0$ and $\beta = -3\pi/4$.

7. Discussion

Motivated by the vision of quantum computation implemented at the device level as a QCA, we have investigated the simplest possible models in one dimension. Although elementary, the No-go Lemma and its proof seem to be original. Evading its conclusion in order to construct a nontrivial QCA led us to the partitioning/alternating evolution rule which, taking the contrapositive of Hénon's dictum,* we interpreted as a quantum particle automaton and then generalized to a QLGA. Although equivalent and similar models have been considered previously as regularizations of quantum field theories [18,19,33], in the probabilistic domain [34], and in the context of hidden variable theories [36], ours seems to be the first unitary simulation.

Decoherence of the quantum state either in memory registers [22] or acted on by logical gates [23] places tight constraints on the number of computational steps which a quantum computer might perform reliably. QCA provide a simple model in which to study decoherence during time evolution. To explore the potential for quantum computation with QCA we are currently simulating decoherence with these models, as well as investigating the possibility of relaxing the homogeneity condition to reflect the presence of local gates/devices/defects, non-periodic boundary conditions, and extension to higher dimensions [30].

These investigations are closely related to several issues in fundamental physics. From the assumptions of discreteness, locality, unitarity, (near) homogeneity and parity invariance we were led to a theory of chiral fermions in one dimension. In fact, the No-go Lemma was named to evoke the well known Nielsen–Ninomiya Theorem concerning the doubling of fermions on the lattice [37], although the logic here is reversed: In $1+1$ dimensions there are several resolutions to the problem [38]; our one component partitioning QCA is equivalent to Casher and Susskind's [39]; reformulating it as a two component QCA with *two* independently evolving fermionic automata as in Section 5 resurrects the problem; and generalizing to the coupled evolution rule given by (18) and (24) is analogous to Wilson's solution [40]. In a more general context than regularizing continuum quantum field theories, the considerations involved here in imposing unitarity and locality on a discrete theory are also relevant to the causal set program for quantum gravity [30,41]. These connections are not surprising: the relation between physics and computation has only been made more intimate by the introduction of quantum mechanics.

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* "Lattice gases are at present often referred to as *cellular automata*. In the present note I wish to advance the thesis that nothing is gained by this practice, and that something is lost." [35].

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